DDW Order and its Role in the Phase Diagram of Extended Hubbard Models

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(Dated: February 1, 2008)

We show in a mean-field calculation that phase diagrams remarkably similar to those recently proposed for the cuprates arise in simple microscopic models of interacting electrons near half-filling. The models are extended Hubbard models with nearest neighbor interaction and correlated hopping. The underdoped region of the phase diagram features $d_{x^2-y^2}$ density-wave (DDW) order. In a certain regime of temperature and doping, DDW order coexists with antiferromagnetic (AF) order. For larger doping, it coexists with $d_{x^2-y^2}$ superconductivity (DSC). While phase diagrams of this form are robust, they are not inevitable. For other reasonable values of the coupling constants, drastically different phase diagrams are obtained. We comment on implications for the cuprates.

PACS numbers: 74.72.-h, 71.10.Hf, 74.25.Dw

I. INTRODUCTION

The high-T_c cuprates exhibit peculiar behavior when underdoped: the density-of-states is depleted at low energies, as if some of the degrees of freedom of the system were developing a gap. This behavior, observed in optical conductivity,[1] NMR,[2] angle-resolved photoemission,[3] c-axis tunneling,[4] and specific heat measurements,[5] was dubbed the 'pseudogap'. The emergence of the 'pseudogap' mimics somewhat the impoverishment of the low-energy excitation spectrum which accompanies the development of $d_{x^2-y^2}$ superconductivity and resembles, more generally, the type of gap formation which is concomitant with a large class of order parameters. However, it does not – at first glance – appear to be connected with the formation of an ordered state. Consequently, it was initially believed that the pseudogap was a crossover phenomenon, and attempts to describe it depended on various approximate methods of treating states with local, fluctuating order.[6,7]

However, it has recently been proposed that the 'pseudogap' state *is* actually a broken-symmetry ordered state, and that the signatures of the order are subtle enough that the state was able to appear incognito.[8,9,10] In Ref. 8, the $d_{x^2-y^2}$ density-wave (DDW) state[11] was advanced as a candidate order. The realization that this is a realistic possibility has led to a re-examination of the experimental circumstances. Recent *elastic* neutron scattering experiments, which directly probe the symmetries broken by DDW order – time-reversal and translation by one lattice spacing – appear to have observed it.[12] A number of other experiments are consistent with the proposal,[8] especially measurements of the superfluid density as a function of doping.[13]

The experimental situation seems promising, which is strong incentive to reconsider the theoretical state of affairs. If the 'pseudogap' state is, indeed, an ordered state, then we should be able to study it within mean-field theory, as we would study the antiferromagnetic state, superconducting state, or any other ordered state. Mean-field theory is unlikely to explain the detailed shape of the phase boundary, but one can hope that it will capture the broad features of the phase diagram, such as its topology and the basic temperature scales. Deep within any phase, with $T \to 0$ and far from any quantum phase transitions, the mean-field Hamiltonian should be the correct Hamiltonian, although the parameters in it may need to be renormalized from their mean-field values. Thus it seems natural to simultaneously study the antiferromagnetic (AF), $d_{x^2-y^2}$ -wave superconducting (DSC), and DDW order parameters in mean-field theory. The interplay and possible coexistence of these orders should be qualitatively and semi-quantitatively explained by mean-field theory. Phase transitions, quantum or thermal, may not be accurately described in their asymptotic limits, but the AF, DDW, and DSC phases will, as will possible phases with coexisting AF, DDW, and DSC orders.

However, there is an immediate problem faced by such a program. What microscopic Hamiltonian should be used? In the early days of high-T_c, it was hoped that the important physics of strong local repulsion and superexchange, which is present in the simplest models, such as the Hubbard and $t-J$ models, would be sufficient to explain all of the interesting physics of the cuprates. This appears not to be the case. Monte Carlo studies have not found superconductivity in the Hubbard model,[14] while Monte Carlo calculations, exact diagonalization, and density-matrix renormalization-group (DMRG) calculations give conflicting results for the $t-J$ model.[15] DMRG studies have found that the behavior of n-leg ladders depends sensitively on the strength of, for instance, second-neighbor hopping,[16] as have Monte Carlo studies.[17] Indeed, some numerical results are sensitively dependent on boundary conditions,[18] which is further indication of the instability of many of these models to relatively small changes in the parameters. Furthermore, the physics of charge-ordering is probably not correctly described by the $t-J$ model without near-neighbor (and

possibly long-range) Coulomb repulsion.[19,20,21] Indeed, it is also clear from experiments that relatively small changes – such as those associated with substituting Nd for La,[22] which is off the radar screen of the $t-J$ and Hubbard models – can radically change at least some aspects of the behavior of these materials. In short, the detailed form of the underlying Hamiltonian matters.

Fortunately, we are not completely in the dark about the nature of the microscopic Hamiltonian. Local Coulomb repulsion, both on-site and near-neighbor, is clearly an important part of the physics. This is known from microscopic calculations of the Hubbard parameters t, U, and also from the fact that the undoped parent compounds are antiferromagnetic insulators. The other important clue – which derives entirely from experiments – is that the cuprates superconduct. The correct microscopic model (or models) must support d-wave superconductivity when doped away from half-filling. If the Hubbard and $t-J$ do not – and it appears that they do not for t/U small – then they cannot describe the cuprates fully.

Our strategy will be to take a generalization of the Hubbard model which includes next-neighbor repulsion and, most importantly, pair-hopping (or correlated hopping). The pair-hopping term favors superconductivity. Even when it is relatively small, it stabilizes superconductivity in the Hubbard model, as we will see. There are a variety of ways in which such a term – or another term with similar effect – could arise, either from quantum chemistry[23,24] or in the passage to an effective description such as the $t-J$ model; in both cases, it is essentially a result of strong local Coulomb repulsion, as superexchange is. In any event, it appears that such physics is necessary to stabilize superconductivity, so we will incorporate it in our model. We will find that such a term also leads to DDW order.

To summarize, we consider a model which is chosen so that it incorporates the basic physics of strong local repulsion *and* so that will have a phase diagram which includes AF at half-filling and DSC at some finite doping. We find that it naturally supports DDW order. In mean-field theory, we find a phase diagram in the temperature-doping plane which resembles the experimental phase diagram of the cuprates, with the DDW phase boundary playing the role of the experimental pseudogap onset line. This DDW line continues into the DSC state, so that the underdoped superconducting state is characterized by both DSC and DDW orders. At low doping, there is also a region of coexistence between AF and DDW orders. We comment on the interpretation of experiments vis-à-vis our findings.

II. MODEL HAMILTONIAN

We consider the following bilayer lattice model of interacting electrons:[25]

$$\mathcal{H} = \mathcal{H}_{\rm kin} + \mathcal{H}_{\rm int}, \tag{1}$$

where

$$\begin{aligned}\mathcal{H}_{\rm kin} = &-t_{ij}\sum_{\langle i,j\rangle}\left(c_{i\sigma}^{(\lambda)\dagger}c_{j\sigma}^{(\lambda)}+{\rm h.c.}\right)\\ &+\frac{t_\perp}{16}\sum_i\Big(c_{i+\hat{x}+\hat{y},\sigma}^{(1)\dagger}c_{i\sigma}^{(2)}+c_{i+\hat{x}-\hat{y},\sigma}^{(1)\dagger}c_{i\sigma}^{(2)}\\ &-c_{i\sigma}^{(1)\dagger}c_{i\sigma}^{(2)}-c_{i+2\hat{x},\sigma}^{(1)\dagger}c_{i\sigma}^{(2)}+x\to y+1\to 2+{\rm h.c.}\Big),\end{aligned} \tag{2}$$

and

$$\begin{aligned}\mathcal{H}_{\rm int} = &U\sum_i n_{i\uparrow}^{(\lambda)}n_{j\downarrow}^{(\lambda)}+V\sum_{\langle i,j\rangle}n_i^{(\lambda)}n_j^{(\lambda)}\\ &-t_c\sum_{\substack{\langle i,j\rangle,\langle i',j\rangle\\ i\neq i'}}c_{i\sigma}^{(\lambda)\dagger}c_{j\sigma}^{(\lambda)}c_{j\sigma}^{(\lambda)\dagger}c_{i'\sigma}^{(\lambda)}.\end{aligned} \tag{3}$$

In the formulas above t_{ij} is hopping with $t_{ij}=t$ for nearest neighbors, $t_{ij}=t'$ for next nearest neighbors and $t_{ij}=0$ otherwise. The other parameters are the tunneling $t_\perp$, the on-site repulsion U, the nearest-neighbor repulsion V, and next-nearest-neighbor correlated hopping t_c. The indices i,j correspond to a lattice site, σ to the spin, and λ to the layer.

The next-nearest-neighbor correlated hopping term is physically kinetic, but since it is also quartic, we are going to treat it as interaction. It hops an electron from i' to j when j is vacated by an electron hopping to i. These two hops are correlated by virtue of Coulomb interaction between the electrons. The presence of this term in the cuprates has been shown in band-structure calculations.[23] Correlated hopping has been discussed in Refs. 24,26,27,28 as a possible mechanism of superconductivity, but it has also been found[25] that it favors DDW order as well.

The tunneling term is momentum conserving.[27,29] We consider a CuO_2 bilayer because the pseudogap has been best characterized in bilayer materials such as YBCO and Bi2212.

To derive a mean-field theory, it is convenient to take the Fourier transform of Eq. (1) and regroup the terms. This task would be particularly simple if there were only one phase at a given set of parameters. For example, a DDW reduced Hamiltonian would look like

$$\mathcal{H}_{\rm DDW} = -g_{\rm DDW}\int_{k,k'} f(k)\,f(k')\,c_{k+Q,\sigma}^{(\lambda)\dagger}c_{k\sigma}^{(\lambda)}c_{k'\sigma'}^{(\lambda)\dagger}c_{k'+Q,\sigma'}^{(\lambda)}, \tag{4}$$

where $f(k)=\cos k_x-\cos k_y$ (the lattice spacing has been set to unit) and the DDW mean-field coupling constant

is

$$g_{\rm DDW} = 8V + 24t_c. \tag{5a}$$

Similar values of the mean filed coupling constants can be derived for other phases as well. Thus, for antiferromagnesm, d-wave superconductivity and (π,π) charge-density wave we derive:

$$g_{\rm AF} = 2U, \tag{5b}$$
$$g_{\rm DSC} = 12t_c - 8V, \tag{5c}$$
$$g_{\rm CDW} = 16V + 24t_c - 2U. \tag{5d}$$

In fact, the interaction part of the Hamiltonian Eq. (3) can be further generalized to include the *interlayer* Coulomb interactions:

$$\mathcal{H}'_{\rm int} = U' \sum_i n_i^{(\lambda)} n_j^{(\lambda')} + V' \sum_{\langle i,j\rangle} n_i^{(\lambda)} n_j^{(\lambda')}, \tag{6}$$

where $\lambda \neq \lambda'$. Then for the given interlayer configuration of the order parameters (antisymmetric for AF and DDW and symmetric for DSC), the mean field coupling constants become:

$$g_{\rm DDW} = 8V + 8V' + 24t_c, \tag{7a}$$
$$g_{\rm AF} = 2U + 2U', \tag{7b}$$
$$g_{\rm DSC} = 12t_c - 8V + 8V'. \tag{7c}$$

For the opposite configuration (symmetric for AF and DDW and antisymmetric for DSC) the contributions of U', V' would be negative, which is the main reason why such configurations have generally higher energy and are not observed. On the other hand, the fact that five interaction terms produce only three phases means that we can have the same phase diagrams (corresponding to a given set of g_p's) for a range of values of the interaction constants. In the following section we will assume that $U' = V' = 0$ so that each phase diagram will correspond to a unique set of U, V, t_c.

The total Hamiltonian contains the reduced parts corresponding to these phases as well as the interactions between the order parameters. However, since we expect $g_{\rm CDW}$ to be negative so that the corresponding order parameter is always zero, we will ignore the term corresponding to this phase. The final form of the reduced Hamiltonian is

$$\begin{aligned}\mathcal{H}_{\rm red} = &\int_k \epsilon_{k\lambda\lambda'} c_{k\sigma}^{(\lambda)\dagger} c_{k\sigma}^{(\lambda')} \\ &- g_{\rm AF} \int_{k,k'} c_{k+Q,\sigma}^{(\lambda)\dagger} c_{k\sigma}^{(\lambda)} c_{k'\sigma'}^{(\lambda)\dagger} c_{k'+Q,\sigma'}^{(\lambda)} \\ &- g_{\rm DDW} \int_{k,k'} f(k) f(k') c_{k+Q,\sigma}^{(\lambda)\dagger} c_{k\sigma}^{(\lambda)} c_{k'\sigma'}^{(\lambda)\dagger} c_{k'+Q,\sigma'}^{(\lambda)} \\ &- g_{\rm DSC} \int_{k,k'} f(k) f(k') c_{k\uparrow}^{(\lambda)\dagger} c_{-k\downarrow}^{(\lambda)\dagger} c_{k'\uparrow}^{(\lambda)} c_{-k'\downarrow}^{(\lambda)}, \end{aligned} \tag{8}$$

where $\epsilon_{k11} = \epsilon_{k22} = \epsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$, $\epsilon_{k12} = \epsilon_{k21} = \epsilon_{k\perp} = (t_\perp/4) f(k)^2$.

The standard Hubbard-Stratonovich mean-field-theoretical treatment of Eq. (8) is to assume the presence of a bosonic mean field, defined as an order parameter, neglect the fluctuations, find the eigenvalues of the Hamiltonian and finally, integrate out the fermion degrees of freedom to derive the free energy.

We define the order parameters of DDW, AF and DSC phases as follows:

$$\phi_\lambda = g_{\rm DDW} \int_k f(k)\, c_{k+Q,\sigma}^{(\lambda)\dagger} c_{k\sigma}^{(\lambda)}, \tag{9a}$$
$$M_\lambda = g_{\rm AF} \int_k c_{k+Q,\sigma}^{(\lambda)\dagger} c_{k\sigma}^{(\lambda)}, \tag{9b}$$
$$\Delta_\lambda = g_{\rm DSC} \int_k f(k)\, c_{k\uparrow}^{(\lambda)\dagger} c_{-k\downarrow}^{(\lambda)\dagger}. \tag{9c}$$

We assume that ϕ_λ and M_λ are anti-symmetric in the bilayer index. Then, the free energy of the system is

$$\begin{aligned} f = &\frac{|M|^2}{g_{\rm AF}} + \frac{|\phi|^2}{g_{\rm DDW}} + \frac{|\Delta|^2}{g_{\rm DSC}} \\ &+ \sum_{s_1,s_2,s_3=\pm1} \int_{\substack{k_x>0\\ k_y>k_x}} \Big[s_1\epsilon_k + s_2\epsilon_{k\perp} - \mu \\ &- 2T \ln\left(2\cosh\left\{\frac{1}{2T}\left[\{f(k)\Delta\}^2 + \left(s_1\left\{[\epsilon_k + s_2\epsilon_{k\perp}]^2 \right.\right.\right.\right. \\ &\left.\left.\left.\left. + [f(k)\phi + s_3 M]^2\right\}^{1/2} - \mu\right)^2\right]^{1/2}\right\}\right)\Big]. \end{aligned} \tag{10}$$

As we expand this expression for small values of the order parameters, we can construct a Landau-Ginzburg theory:

$$\begin{aligned} f(T) = f_0(T) + \sum_p a_p |\Phi_p|^2 + \sum_p b_p |\Phi_p|^4 \\ + \sum_{p\neq p'} c_{pp'} |\Phi_p|^2 |\Phi_{p'}|^2, \end{aligned} \tag{11}$$

where p denotes the kind of the order parameter (AF, DDW or DSC) and Φ_p is the order parameter (M, ϕ or Δ, respectively). The a_p coefficients cross zero at the transitions so that $a_p = 0$ are the equations that determine critical temperature T_c:

$$a_p = \frac{1}{g_p} - \sum_{s_1,s_2,s_3=\pm1} \int_{\substack{k_x>0\\ k_y>k_x}} K_p(k), \tag{12}$$

where

$$K_{\rm AF}(k) = \frac{1}{2|\bar\epsilon_k|} \tanh\left(\frac{|s_1\bar\epsilon_k - \mu|}{2T}\right), \tag{13a}$$
$$K_{\rm DDW}(k) = f(k)^2 K_{\rm AF}(k), \tag{13b}$$
$$K_{\rm DSC}(k) = \frac{f(k)^2}{2|s_1\bar\epsilon_k - \mu|} \tanh\left(\frac{|s_1\bar\epsilon_k - \mu|}{2T}\right). \tag{13c}$$

Here $\bar{\epsilon}_k = \epsilon_k + s_2\epsilon_{k\perp}$. The b_p coefficients are positive:

$$b_p = \sum_{s_1,s_2,s_3=\pm 1} \int_{\substack{k_x>0 \\ k_y>k_x}} K'_p(k), \tag{14}$$

where

$$K'_{\mathrm{AF}}(k) = \frac{\eta_1(k)}{8\left|\bar{\epsilon}_k\right|^3}, \tag{15a}$$

$$K'_{\mathrm{DDW}}(k) = f(k)^4 K'_{\mathrm{AF}}(k), \tag{15b}$$

$$K'_{\mathrm{DSC}}(k) = \frac{f(k)^4 \eta_2(k)}{8\left|s_1\bar{\epsilon}_k - \mu\right|^3}, \tag{15c}$$

where

$$\eta_1(k) = \tanh\left(\frac{|s_1\bar{\epsilon}_k - \mu|}{2T}\right) - \frac{|\bar{\epsilon}_k|/2T}{\cosh\left(\frac{|s_1\bar{\epsilon}_k-\mu|}{2T}\right)^2}, \tag{16a}$$

$$\eta_2(k) = \tanh\left(\frac{|s_1\bar{\epsilon}_k - \mu|}{2T}\right) - \frac{|s_1\bar{\epsilon}_k - \mu|/2T}{\cosh\left(\frac{|s_1\bar{\epsilon}_k-\mu|}{2T}\right)^2}. \tag{16b}$$

Finally, the $c_{pp'}$ coefficients are

$$c_{pp'} = \sum_{s_1,s_2,s_3=\pm 1} \int_{\substack{k_x>0 \\ k_y>k_x}} K''_{pp'}(k), \tag{17}$$

where

$$K''_{\mathrm{AF,DSC}}(k) = \frac{f(k)^2}{4\left|s_1\bar{\epsilon}_k - \mu\right|^2\left|\bar{\epsilon}_k\right|}\eta_2(k), \tag{18a}$$

$$K''_{\mathrm{DDW,DSC}} = f(k)^2 K''_{\mathrm{AF,DSC}}(k), \tag{18b}$$

$$K''_{\mathrm{AF,DDW}}(k) = \frac{3f(k)^2}{4\left|\bar{\epsilon}_k\right|^3}\eta_1(k). \tag{18c}$$

The fact that all $K''_{pp'} > 0$ implies that the phases compete with each other.

III. PHASE DIAGRAM

The mean field phase diagram can be derived by minimizing Eq. (10) at fixed doping.

Since there is a large number of parameters in our model, there is substantial variety in the possible diagrams. One such diagram, generated with $t = 0.5$ eV, $t' = -0.025$ eV, $t_\perp = 0.05$ eV, $g_{\mathrm{AF}} = 0.06$ eV, $g_{\mathrm{DDW}} = 0.02$ eV, $g_{\mathrm{DSC}} = 0.01$ eV, is shown on the figure 1. The corresponding values of the interaction constants are $U \simeq 0.03$ eV, $V = 0$ eV, $t_c \simeq 0.8 \times 10^{-3}$ eV. Note that for these values of the constants, $g_{\mathrm{CDW}} = -0.04$ eV < 0, which is consistent with our assumption that a (π, π) charge-density wave is not energetically favorable.

Another diagram, shown on the figure 2, was generated with $t = 0.5$ eV, $t' = 0$, $t_\perp = 0.1$ eV, $g_{\mathrm{AF}} = 0.084$ eV, $g_{\mathrm{DDW}} = 0.038$ eV, and $g_{\mathrm{DSC}} = 0.017$ eV. The corresponding values of the interaction constants are $U \simeq 0.042$ eV, $V \simeq 1.7 \times 10^{-4}$ eV, $t_c \simeq 1.5 \times 10^{-3}$ eV, and also $g_{\mathrm{CDW}} \simeq -0.045$ eV.

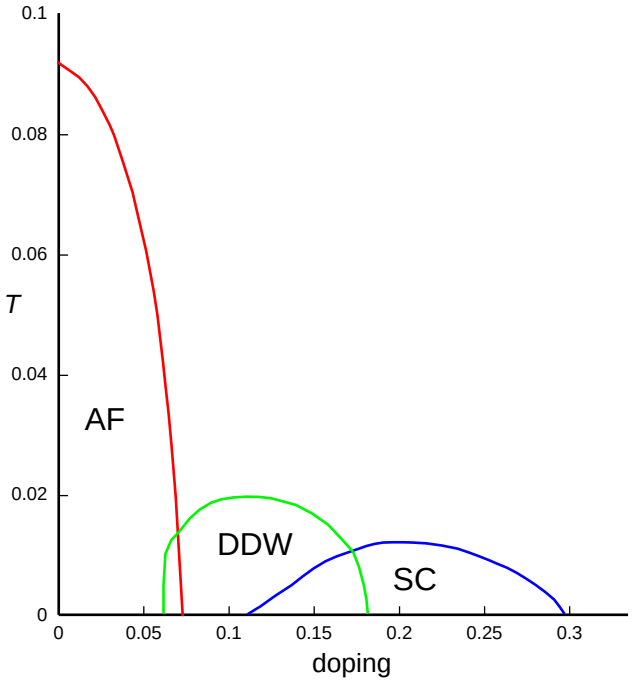

FIG. 1: Phase diagram for $t = 0.5$ eV, $t' = -0.025$, $t_\perp = 0.05$ eV, $U \simeq 0.03$ eV, $V = 0$ eV, $t_c \simeq 0.8 \times 10^{-3}$ eV. ($g_{\mathrm{AF}} = 0.06$ eV, $g_{\mathrm{DDW}} = 0.02$ eV, $g_{\mathrm{DSC}} = 0.01$ eV.)

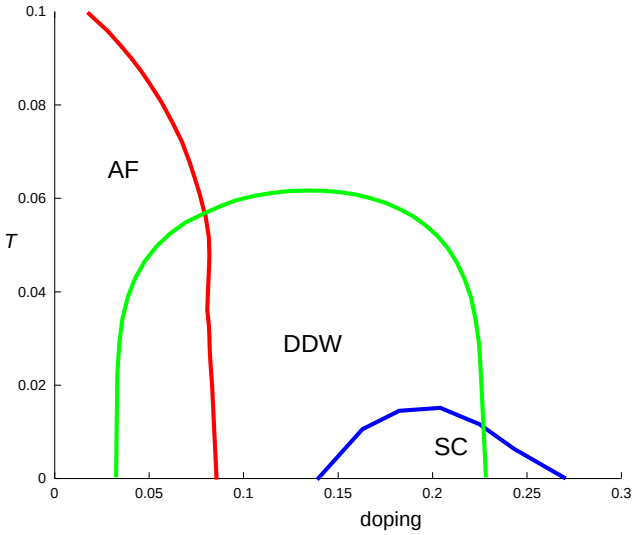

FIG. 2: Phase diagram for $t = 0.5$ eV, $t' = 0$, $t_\perp = 0.1$ eV, $U \simeq 0.042$ eV, $V \simeq 1.7 \times 10^{-4}$ eV, $t_c \simeq 1.5 \times 10^{-3}$ eV. ($g_{\mathrm{AF}} = 0.084$ eV, $g_{\mathrm{DDW}} = 0.038$ eV, $g_{\mathrm{DSC}} = 0.017$ eV.)

As we can see, in both diagrams the antiferromagnetic transition temperature at half-filling is close to 1000 K. This should be understood as the scale at which two-dimensional antiferromagnetic correlations develop locally. Due to the Mermin-Wagner-Coleman theorem, which states that a continuous symmetry cannot be bro-

ken spontaneously at finite-temperature in $2D$, the transition temperature is zero for a single bilayer. The coupling between different bilayers (which is not included in our single-bilayer calculation) stabilizes the antiferromagnetic phase with a transition temperature around 410 K. In lightly-doped cuprates, the presence of impurities causes the misalignment of locally ordered antiferromagnetic clusters, thereby forming a spin glass. Thus, if we interpret our T_N as the scale of local $2D$ antiferromagnetic order, which could become $3D$ antiferromagnetic order or spin glass order, then the phase diagrams of Figs. 1 and 2 are very reasonable, indeed.

Experiments might lead us to expect that DDW order would occur in the range of doping between 0.07 and 0.19. This range is smaller than one shown on Fig. 2 and a bit larger than that shown in Fig. 1. The temperature scale for this phase on Fig. 1 is very reasonable; it is almost three times higher on Fig. 2. This change occurred primarily as a result of the increased value of t_c. If we further increase t_c to 1.9×10^{-3} eV, the DDW phase will begin to suppress the AF phase and will expand up to half-filling at finite temperatures. In general, varying the interaction constants by less that 20 – 30% does not change the phase diagram qualitatively. However, larger variations lead to completely different classes of phase diagrams, such as those with the AF phase suppressed or without a DDW phase at all. For example, Fig. 3 shows the case when due to the smaller value of correlation hopping, both DDW and DSC phases disappear and only AF phase remains in the diagram.

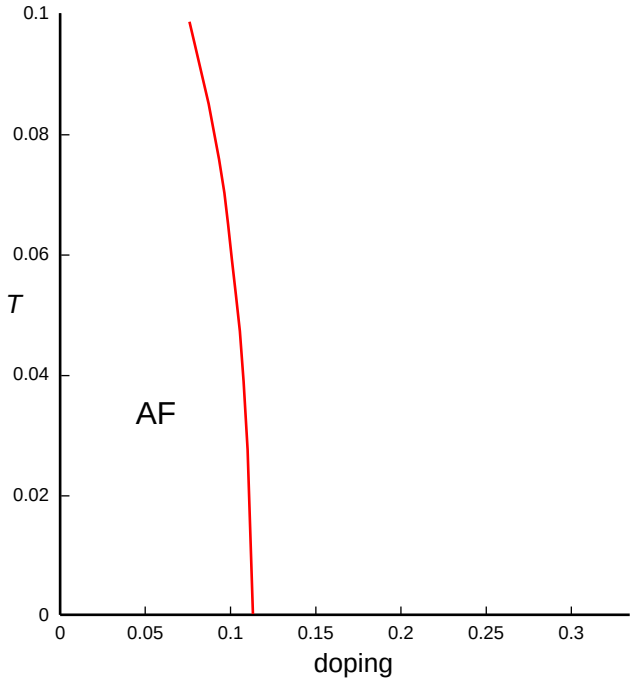

FIG. 3: Phase diagram for $t = 0.5$ eV, $t' = -0.025$, $t_\perp = 0.05$ eV, $U = 0.05$ eV, $V = 0$ eV, $t_c \simeq 3.3 \times 10^{-4}$ eV. ($g_{\rm AF} = 0.1$ eV, $g_{\rm DDW} = 0.008$ eV, $g_{\rm DSC} = 0.004$ eV.)

The DSC phase occupies a doping range away from half-filling primarily as a result of band structure effects associated with the bilayer splitting. In the absence of other orders, it would extend all the way to half-filling, but it is suppressed at low doping by DDW and AF order. In a more realistic calculation, superconductivity would be suppressed close to half-filling by no-double-occupancy constraint, i.e. by strong local Coulomb repulsion. However, the DSC phase never even makes it that close to half-filling because the DDW phase intervenes.

An important feature common to both diagrams is the existence of regions with two simultaneous kinds of order. Namely, there is a region with DDW+AF order and a region with DDW+DSC order. The system is an insulator in the AF state at half-filling, a metal in the DDW and DDW+AF states, and a superconductor in the DSC and DDW+DSC states.

All of the transitions are of second order at the mean-field level because of the signs of the $c_{pp'}$ couplings between the order parameters in the Ginzburg-Landau theory Eq. (11).

The calculated dependence of the chemical potential μ on the doping x inside the DDW phase and in its proximity is nonmonotonic. This is due to the rapid development of the DDW gap, which causes the chemical potential to be lower than in the normal state. The thermodynamic inequality $(\partial\mu/\partial x)_{T,V} \leq 0$ implies that when this is violated, mean-field theory should be corrected using Maxwell's construction, which signals that fluctuations drive the transitions first-order as a function of μ. Consequently, we would expect the underdoped side of the DSC phase to be characterized by a smaller than expected chemical shift, as has been observed.[30] A first-order phase transition as a function of chemical potential is manifested as phase separation in a two-phase coexistence region spanning a range of dopings when the doping is held fixed instead. It has been argued that such phase separation will be precluded by Coulomb interactions, thereby leading to stripe formation.[19,20]

IV. CONCLUSION

We have studied the phase diagram of a bilayer lattice model using mean field theory. Since we have focused on ordered phases, this should be a valid approximation. We found that for certain ranges of the values of the interaction constants the phase diagram agrees well with the experimentally observed phase diagram of YBCO if the 'pseudogap' is associated with DDW order. The diagram remains in qualitative agreement with the experimental data when the parameters of our model vary by less than 20 – 30% and becomes qualitatively different for larger variations. Clearly, such a phase diagram is reasonably robust, but is hardly inevitable. This is reassuring because high-temperature superconductivity is stable, but only appears in a special class of materials (to the best

of our current knowledge).

There are some systematic errors associated with mean-field theory, on which we now comment. It underestimates the effect of fluctuations. Thus, the Néel temperature is very large in mean-field theory, while it should actually be zero in any strictly two-dimensional system. However, the Néel temperature which we find should be regarded as the temperature below which a renormalized classical description is valid.[31] The Néel temperature observed in experiments is associated with the crossover from 2D to 3D. Mean-field theory also overestimates the coupling which drives antiferromagnetism, which it takes to be essentially U. For small U, this is correct, but for large U, it should be replaced by $J \sim t^2/U$. Indeed, the large-U limit is generally somewhat problematic near half-filling since the Gutwiller constraint is not enforced in mean-field theory. The $d_{x^2-y^2}$ symmetry of the DDW and DSC states lead one to the erroneous conclusion that they are completely unaffected by large U. This cannot, of course, really be true; clearly, mean-field theory underestimates the tendency of large-U to push these ordered states away from half-filling. The seemingly small value of U taken in our calculation should be interpreted in light of these observations. Other mean-field treatments which incoporate strong local Coulomb repulsion more prominently have also found DDW order in a generalization of the $t-J$ model[32] and in the Hubbard model with nearest neighbor attraction.[33]

We find that the scale associated with superconductivity is largely determined by the strength of correlated hopping. At the moment, this is rather *ad hoc*, but we had little choice but to introduce some term of this sort in order to have a phase diagram which includes superconductivity. It is possible that the superexchange coupling J plays a more important role than we have accorded it in setting T_c, but superexchange is beyond a mean-field treatment.

As we have seen, the very term which stabilizes superconductivity also supports the development of DDW order. One way of interpreting our results begins with the observation that the DDW order parameter, when combined with the real and imaginary parts of the DSC order parameter form a triplet under an $SU(2)$ group of transformations.[25,34] If this 'pseudospin' $SU(2)$ is a symmetry of the Hamiltonian, then DDW and DSC orders will be equally favored. Thus, one can envision that the important order-producing term in the Hamiltonian is $SU(2)$-symmetric while small symmetry-breaking terms drive the system into either the DDW or DSC states. Our result shows that pair-hopping is of this form. Are all physically reasonable mechanisms for $d_{x^2-y^2}$ superconductivity similarly invariant under pseudospin $SU(2)$? This is an open problem; we have answered in the affirmative for one particular class of Hamiltonians.

Acknowledgments

We would like to thank S. Chakravarty for discussions. C.N. is supported by the National Science Foundation under Grant No. DMR-9983544 and by the Alfred P. Sloan Foundation. E.P. is supported in part by the Department of Energy under grant DE-FG03-92-ER 40701.

[1] J. Orenstein *et al.*, Phys. Rev. B **42**, 6342 (1990); A. Puchkov *et al.*, J. Phys. Cond. Matt., **8**, 10049 (1996).
[2] H. Yasuoka, T. Imai, and T. Shimizu, in *Strong Correlations and Superconductivity*, edited by H. Fukuyama, S. Maekawa, and A. P. Malozemoff (Springer-Verlag, 1989); N. J. Curro *et al.*, Phys. Rev. Lett. **85**, 642 (2000).
[3] J. Harris *et al.*, Nature **382**, 51 (1996); M. R. Norman *et al.*, Nature **392**, 157 (1998).
[4] M. Kugler *et al.*, Phys. Rev. Lett. **86**, 4911 (2001).
[5] J. L. Tallon and J. W. Loram, Physica C **349**, 53 (2001).
[6] V. J. Emery and S. A. Kivelson, Nature **374**, 434 (1995); M. Randeria, in *Proceedings of the Tenth International School of Physics "Enrico Fermi", Varenna, 1997*, edited by G. Iadonisi and J. R. Schrieffer (IOS Press, Amsterdam, 1998).
[7] X.-G. Wen and P. A. Lee, Phys. Rev. Lett. **76**, 503 (1996).
[8] S. Chakravarty, R. B. Laughlin, D. K. Morr, and C. Nayak, Phys. Rev. B **63**, 4503 (2001).
[9] C. M. Varma, Phys. Rev. Lett. **83**, 3538 (1999).
[10] S. Kivelson, E. Fradkin, and V. Emery, Nature **393**, 550 (1998).
[11] H. J. Schulz, Phys. Rev. B **39**, 2940 (1989); I. Affleck and J. B. Marston, Phys. Rev. B **37**, 3774 (1988); G. Kotliar, Phys. Rev. B **37**, 3664 (1988); D. A. Ivanov, P. A. Lee, and X.-G. Wen, Phys. Rev. Lett. **84**, 3958 (2000).
[12] H. Mook, P. Dai, and F. Dogan, Phys. Rev. B **64**, 012502 (2001); H. Mook *et al.*, in preparation. For a theoretical discussion of the experiments, see S. Chakravarty, H.-Y. Kee, and C. Nayak, Int. J. Mod. Phys. **15**, 2901 (2001); cond-mat/0112109; see also the earlier work by T. Hsu, J. B. Marston, and I. Affleck, Phys. Rev. Lett. **43**, 2866 (1991).
[13] Y. J. Uemura *et al.*, Phys. Rev. Lett. **62**, 2317(1989).
[14] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994); A. Moreo, Phys. Rev. B **45**, 5059 (1992); S. Zhang, J. Carlson, and J. E. Gubernatis, Phys. Rev. B **55**, 7464 (1997).
[15] T. Tohyama *et al.*, Phys. Rev. B **58**, R11649 (1999); S. R. White and D. J. Scalapino, Phys. Rev. Lett. **80**, 1272 (1998); S. Sorella *et al.*, cond-mat/0110460.
[16] S. R. White and D. J. Scalapino, Phys. Rev. B **60**, R753 (1999).
[17] D. Poilblanc *et al.*, Phys. Rev. B **62**, R14633 (1999).
[18] S. C. Hellberg and E. Manousakis, Phys. Rev. Lett. **83**, 132 (1999).
[19] S. A. Kivelson and V. J. Emery, Synthetic Metals, **80**, 151 (1996); Phys. Rev. Lett. **74**, 3253 (1995); and references therein.
[20] J. Zaanen, Physica C **317 - 318**, 217 (1999), and references therein.
[21] E. Arrigoni *et al.*, cond-mat/0012293.
[22] J. M. Tranquada *et al.*, Nature **375**, 561 (1995); Phys. Rev. B **54**, 7489 (1996).

[23] J. Appel, M. Grodzicki, and F. Paulsen, Phys. Rev. B **47**, 2812 (1993); O. Navarro and C. Wang, Sol. State Commun. **83**, 473 (1992).
[24] J. E. Hirsch, Physica C **58**, 326 (1989).
[25] C. Nayak, Phys. Rev. B **62**, 4880 (2000).
[26] J. Wheatley, T. Hsu, and P. Anderson, Phys. Rev. B **37**, 5897 (1988).
[27] S. Chakravarty, A. Sudbø, P. Anderson, and S. Strong, Science **261**, 337 (1993).
[28] F. Assaad, M. Imada, and D. Scalapino, Phys. Rev. B **56**, 15001 (1997).
[29] O. K. Andersen, A. I. Liechtenstein, O. Jepsen, and F. Paulsen, J. Phys. Chem. Solids **56**, 1573 (1995).
[30] A. Ino *et al.*, Phys. Rev. Lett. **79**, 2101 (1997).
[31] S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. B **39**, 2344 (1989).
[32] E. Cappelluti and R. Zeyher, Phys. Rev. B **59**, 6475 (1999).
[33] T. Stanescu and P. Phillips, Phys. Rev. B **64**, 220509/1-4 (2001).
[34] C. Nayak, Phys. Rev. B **62**, R6135 (2000).